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*Form Approved
OMB No. 0704-0188*

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|--|--|---|--|-----------------------------------|--|
| 1. REPORT DATE (DD-MM-YYYY) | | 2. REPORT TYPE Technical Papers | | 3. DATES COVERED (From - To) | |
| | | | | | |
| 4. TITLE AND SUBTITLE | | | | 5c. PROGRAM ELEMENT NUMBER | 5d. PROJECT NUMBER <i>2303</i> |
| 6. AUTHOR(S) | | | | 5e. TASK NUMBER <i>M2C8</i> | 5f. WORK UNIT NUMBER |
| 7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) Air Force Research Laboratory (AFMC) AFRL/PRS 5 Pollux Drive Edwards AFB CA 93524-7048 | | | | 8. PERFORMING ORGANIZATION REPORT | |
| 9. SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES) Air Force Research Laboratory (AFMC) AFRL/PRS 5 Pollux Drive Edwards AFB CA 93524-7048 | | | | | |
| 12. DISTRIBUTION / AVAILABILITY STATEMENT Approved for public release; distribution unlimited. | | | | | |
| 13. SUPPLEMENTARY NOTES | | | | | |
| 14. ABSTRACT | | | | | |
| 15. SUBJECT TERMS | | | | | |
| 16. SECURITY CLASSIFICATION OF: | | | 17. LIMITATION OF ABSTRACT <i>A</i> | 18. NUMBER OF PAGES | 19a. NAME OF RESPONSIBLE PERSON Leilani Richardson |
| a. REPORT <i>Unclassified</i> | b. ABSTRACT <i>Unclassified</i> | c. THIS PAGE <i>Unclassified</i> | | | 19b. TELEPHONE NUMBER (include area code) (661) 275-5015 |

20021212 094

CS

MEMORANDUM FOR PR (Contractor/In-House Publication)

FROM: PROI (TI) (STINFO)

18 Apr 2000

SUBJECT: Authorization for Release of Technical Information, Control Number: **AFRL-PR-ED-AB-2000-075**
Vij, V., Boatz, J.A., Tham, F., Vij, A., and Christe, K.O., "On the Lewis Acidity of LiF" (Abstract)

16th International Symposium of Fluorine Chemistry (Statement A)
(Durham, UK, 23 Jul 00) (Submission Deadline: 18 Apr 2000)

1. This request has been reviewed by the Foreign Disclosure Office for: a.) appropriateness of distribution statement, b.) military/national critical technology, c.) export controls or distribution restrictions, d.) appropriateness for release to a foreign nation, and e.) technical sensitivity and/or economic sensitivity.

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PHILIP A. KESSEL
Technical Advisor
Propulsion Science and Advanced Concepts Division

Date

Oral Presentation Preferred

Participant

ON THE LEWIS ACIDITY OF LiF

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Based on the recently developed pF⁻ Lewis acidity scale,¹ free gaseous LiF is a surprisingly strong Lewis acid, comparable to SiF₄. It was therefore of interest to study whether a strong Lewis base, such as CsF, could transfer a fluoride ion to LiF with formation of a LiF₂⁻ anion. Theoretical calculations were carried out for LiF₂⁻ and show that free gaseous LiF₂⁻ is a linear, vibrationally stable species. Furthermore, the phase-diagram of the LiF/CsF system shows a eutectic at a 1:1 mole ratio that gives a distinct X-ray powder diffraction pattern.² We have prepared this eutectic by fusion of a 1:1 mixture of LiF and CsF in a platinum crucible. Single crystals were obtained by slow cooling of the melt in a dry nitrogen stream. The resulting product was characterized by vibrational spectroscopy, and its crystal structure was determined. It is shown that CsLiF₂ does not contain isolated LiF₂⁻ anions, but exhibits an interesting three-dimensional network of alternating tetra-coordinated LiF₄ and octa-coordinated CsF₈ units.

1. K. O. Christe, D. A. Dixon, D. McLemore, W. W. Wilson, J. A. Sheehy and J. A. Boatz, *J. Fluorine Chem.*, 2000, **101**, 151.
2. D. L. Deadmore and J. S. Machin, *J. Phys. Chem.*, 1960, **64**, 824.